Journal of Computational and Applied Mathematics 18 (1987) 235–247
North-Holland

Spline-Gauss rules and the Nyström method for solving integral equations in quantum scattering

L. PRETORIUS and D. EYRE
National Research Institute for Mathematical Sciences of the CSIR, P.O. Box 395, Pretoria 0001, Republic of South Africa

Received 10 January 1986
Revised 1 April 1986

Abstract: This paper is concerned with an n-point Gauss quadrature

$$\int_{-1}^{1} g(t)\,\mathrm{d}t \approx \sum_{j=1}^{n} g(t_{n,j})w_{n,j}, \quad g \in C[-1,1],$$

where the points $\{t_{n,j}\}_{j=1}^{n}$ and weights $\{w_{n,j}\}_{j=1}^{n}$ are chosen to be exact when g is defined on a $2n$-dimensional space of polynomial splines. The spline-Gauss quadrature is used in a Nyström method for solving integral equations of the second kind. A practical application is provided by solving integral equations that arise in quantum scattering theory.

Keywords: Integral equations, Gauss quadrature, B-splines.

1. Introduction

This paper describes a method for constructing a Gauss quadrature formula that is exact for splines. The numerical utility of the spline-Gauss quadrature is investigated by solving an integral equation of the second kind [2]

$$f(s) = y(s) - \int_{-1}^{1} K(s,t)f(t)\,\mathrm{d}t, \quad -1 \leqslant s \leqslant 1, \tag{1.1}$$

where the inhomogeneous term y and the kernel K are given. For this purpose we employ an approximation method due to Nyström [17] as well as an iterative variation of the Nyström method due to Brackhage [6].

Gauss quadrature formulas are characterized by the approximation

$$\int_{-1}^{1} g(t)\,\mathrm{d}t \approx \sum_{j=1}^{n} g(t_{n,j})w_{n,j}, \tag{1.2}$$

where the points $\{t_{n,j}\}_{j=1}^{n}$ and weights $\{w_{n,j}\}_{j=1}^{n}$ are exact for a function g that is given by a linear combination of $2n$ basis functions $\{\phi_{2n,i}\}_{i=1}^{2n}$. (The important feature of Gauss quadrature is that it is exact for $2n$ basis functions. Ordinary quadrature is exact only for n basis functions.)

Much of the practical application of Gauss quadrature has been limited to the use of orthogonal polynomials [8,20]. In other words, the basis functions have been chosen to be global elements. On the other hand, it is known that finite elements, which employ piecewise polynomials such as splines [4], possess good interpolation properties. A second advantage of using finite elements, rather than global elements, is that it is often possible to construct a general algorithm for solving equations. It would appear, therefore, that a numerical investigation of spline-Gauss quadrature for solving equations (in the present case integral equations) may provide some insight into the possible usefulness of such approximations. As far as we are aware, this is the first time that spline-Gauss quadrature has been applied to a physical problem. The problem we shall consider is the numerical treatment of an integral equation that describes quantum scattering.

One reason why spline-Gauss quadrature has received little attention is because the strong theory of orthogonal polynomials that is fundamental to the construction of well-known Gauss quadrature formulas for polynomials does not apply in the case of spline functions.

As B-splines are easy to work with, they have been suggested as a suitable basis for treating the integral equation (1.1) [1,12]. In the present paper we construct a Gauss quadrature that is exact for B-splines. Hence our numerical approach permits an application of the Nyström method using Gauss quadrature, while at the same time retaining the advantage of spline interpolation.

We remark that although the Nyström method using spline quadrature has been the subject of numerous investigations for solving integral equation (1.1) with continuous kernel [15], the use of Gauss quadrature for splines has not. We have, therefore, as part of our numerical investigation, made a comparison of the Nyström method with spline quadrature and Gauss quadrature.

In our numerical examples we have considered only uniformly spaced knots. (Of course, the Gauss points $\{t_{n,j}\}_{j=1}^{n}$ are not uniformly spaced.) While a uniform distribution of knots is not essential for our numerical method, it does lead to a simpler algorithm. We defer the extension to non-uniformly spaced knots for future work.

In the case of quantum scattering the integral equation (1.1) may have a singular kernel [9]. A standard technique if the kernel has a weak singularity, for example logarithmic [9], is to use product integration [1,2]. In our case, however, the kernel has a Cauchy principal value singularity. We employ a modification [10] of the original Nyström technique to construct a solvable system of equations.

Section 2 describes our numerical method. We construct a Gauss quadrature rule for splines, and apply the Nyström method to equation (1.1) for the case of a continuous kernel. We provide a theoretical estimate of the rates of convergence for the approximation method. Section 3 is devoted to an integral equation taken from scattering theory. We employ the method of Haftel and Tabakin to treat integral equations with singular kernel of the Cauchy principal value type. Section 4 gives our numerical results and discussion.

2. Approximation method

The main purpose of this section is to describe our numerical method for constructing spline-Gauss quadrature. We show how Gauss quadrature may be used for solving integral equation (1.1) in the case of a continuous kernel. In the following section we relax the

smoothness condition on the kernel and treat the physically interesting case when the kernel in equation (1.1) contains a Cauchy principal value singularity.

2.1. Gauss quadrature for splines

The existence of Gauss-type quadrature formulas for spline functions is guaranteed by the following theorem [13].

Existence Theorem. *There exists an n-point Gauss quadrature formula (see equation* (1.2)) *where* $-1 < t_{n,1} < t_{n,2} < \cdots < t_{n,n} < 1$, $w_{n,j} > 0$, $j = 1, 2, \ldots, n$ *that is exact for every spline function of the form*

$$s(t) = \sum_{i=0}^{l} a_i t^i + \sum_{i=1}^{r} b_i (t - z_i)_+^l, \tag{2.1}$$

where $-1 < z_1 < z_2 < \cdots < z_r < 1$, $t_+ = \max(0, t)$, *provided that* $l + r + 1 = 2n$.

This theorem implies that for a given number of knots r, the number of quadrature points used in a Gauss quadrature formula is $\frac{1}{2}(r + l + 1)$. Since $l + 1$ is the order of the spline, which we assume to be small compared to r, then the number of quadrature points is approximately half the number of knots in the integration interval. The uniqueness of this Gauss quadrature formula follows from [14, theorem 3.4].

The algebraic method [8] for constructing Gauss quadrature formulas for orthogonal polynomials may be generalized for spline functions. In this case an n-point Gauss quadrature is constructed by solving a $2n$-dimensional non-linear system of algebraic equations for the $2n$ unknowns $\{t_{n,k}\}_{k=1}^{n}$ and $\{w_{n,k}\}_{k=1}^{n}$. The moment equations to be solved are

$$\sum_{k=1}^{n} w_{n,k} \phi_{2n,j}(t_{n,k}) = \int_{-1}^{1} \phi_{2n,j}(t)\, \mathrm{d}t, \quad j = 1, 2, \ldots, 2n, \tag{2.2}$$

with $\phi_{2n,j}(t) = t^{j-1}$, $j = 1, 2, \ldots, l + 1$ and $\phi_{2n,j}(t) = (t - z_i)_+^l$, $i = 1, 2, \ldots, r$.

Since we must solve a non-linear system, it is useful to reduce the dimension of this system by exploiting symmetry. It is well known that for an integral of the form

$$\int_{-1}^{1} g(t) w(t)\, \mathrm{d}t, \tag{2.3}$$

with a symmetric weight function $w(t)$, which in our case is identically 1, the Gauss points $\{t_{n,k}\}_{k=1}^{n}$ are located symmetrically in $[-1, 1]$, and the weights corresponding to symmetric points are equal. Therefore

$$w_{n,k} = w_{n,n-k+1}, \quad t_{n,k} = -t_{n,n-k+1}, \qquad k = 1, 2, \ldots, \lfloor \tfrac{1}{2} n \rfloor. \tag{2.4}$$

If n is odd, $t_{n,(n+1)/2} = 0$. For simplicity we also assume that the knots $\{z_i\}_i^r = 1$ are uniformly spaced and therefore symmetrically located in $[-1, 1]$.

Using the above symmetry, we obtain the following n-dimensional system: The first equation is either

$$\sum_{k=1}^{n/2} w_{n,k} = 1 \quad (n \text{ even}),$$

or

$$\sum_{k=1}^{(n-1)/2} w_{n,k} + \tfrac{1}{2} w_{n,(n+1)/2} = 1 \quad (n \text{ odd}), \tag{2.5}$$

and the remaining equations are

$$\sum_{k=1}^{N} w_{n,k} t_{n,k}^2 = \tfrac{1}{3}, \quad \ldots, \quad \sum_{k=1}^{N} w_{n,k} t_{n,k}^{l-1} = \frac{1}{l},$$
$$\sum_{k=1}^{N} w_{n,k} (t_{n,k} - z_i)_+^l = \frac{1}{(l+1)} (1 - z_i)^{l+1}, \quad i = 1, 2, \ldots, \tfrac{1}{2}r, \tag{2.6}$$

where $N = \frac{1}{2}n$ (n even) or $N = \frac{1}{2}(n-1)$ (n odd), and $z_i = -1 + 2i/(2n-l)$, $i = 1, 2, \ldots, \frac{1}{2}r = \frac{1}{2}(2n-1-1)$.

We now consider convergence properties of the spline-Gauss quadrature rule. For brevity we write equation (1.2) as

$$Ig \approx Q_n g. \tag{2.7}$$

We use the following notation [4]:

(i) $S_{l+1,z}$ is the collection of all linear combinations of B-splines of order $l+1$ for the knot sequence $z = \{z_i\}_{i=-l}^{2n}$;
(ii) $\operatorname{dist}(g, S) = \min_{s \in S}\{\|g - s\|\}$, the distance of $g \in C[a, b]$ from the subset $S \subset C[a, b]$;
(iii) $\|g\| = \max_{a \leqslant t \leqslant b}\{|g(t)|\}$, the uniform norm of $g \in C[a, b]$;
(iv) h_z is the grid size associated with z.

Convergence Theorem. *Let $g \in C^{(l)}[-1, 1]$. Then for some constant C_{l+1}*

$$\operatorname{dist}(Ig, Q_n g) \leqslant C_{l+1} \|g^{(l+1)}\| h_z^{l+1}. \tag{2.8}$$

This means that the distance of Ig (where g is a smooth function) from $Q_n g$ goes to zero at least as fast as the $(l+1)$th power of the grid size h_z.

Proof. From theorem XII · I [14, p.170] it follows that for some constant $\tilde{C}_{l+1}$,

$$\operatorname{dist}(g, S_{l+1,z}) \leqslant \tilde{C}_{l+1} \|g^{(l+1)}\| h_z^{l+1}. \tag{2.9}$$

For $s \in S_{l+1,z}$ we know that $Q_n S = Is$ since Q_n is exact for $S_{l+1,z}$, and therefore,

$$\begin{aligned} \operatorname{dist}(Ig, Q_n g) &= |(Ig, Q_n g)| \\ &\leqslant |Ig - Is| + |Is - Q_n g| = |Ig - Is| + |Q_n g - Q_n s|. \end{aligned} \tag{2.10}$$

By definition

$$Q_n g = \sum_{i=1}^{n} w_i g(t_i), \quad t_i \in (-1, 1),$$

and hence,

$$|Q_n g| \leqslant \sum_{i=1}^{n} w_k |g(t_i)| = Q_n |g|, \tag{2.11}$$

and by (2.5),

$$\sum_{i=1}^{n} w_i = 2. \tag{2.12}$$

Therefore,

$$\begin{aligned} \operatorname{dist}(Ig, Q_n g) &\leqslant 2 \max_{-1 \leqslant t \leqslant 1} |g(t) - s(t)| + 2 \max_{-1 \leqslant t \leqslant 1} |g(t) - s(t)| \\ &= 4\|g - s\| \quad \forall s \in S_{l+1,z} \\ &\leqslant 4 \min_{s \in S_{l+1,z}} \|g - s\| \end{aligned} \tag{2.13}$$

by inequality (2.9).
We therefore have the upper bound

$$\operatorname{dist}(Ig, Q_n g) \leqslant C_{l+1} \|g^{(l+1)}\| h_z^{l+1} \tag{2.14}$$

where $C_{l+1} = 4\tilde{C}_{l+1}$.

2.2. Nyström method

Let $\{t_{n,j}\}_{j=1}^{n}$ and $\{w_{n,j}\}_{j=1}^{n}$ be the given points and weights in our n-point quadrature formula. An approximation to the integral in equation (1.1) is obtained by replacing the kernel operator $\mathscr{K}$, defined by

$$\mathscr{K}g(s) = \int_{-1}^{1} K(s, t) g(t)\, dt, \tag{2.15}$$

with the approximation

$$\mathscr{K}_n g(s) = \sum_{j=1}^{n} K(s, t_{n,j}) g(t_{n,j}) w_{n,j}. \tag{2.16}$$

In this way we obtain an approximation $f_n(s)$ to equation (1.1) that satisfies

$$f_n(s) = y(s) - \sum_{j=1}^{n} K(s, t_{n,j}) f_n(t_{n,j}) w_{n,j}. \tag{2.17}$$

The Nyström method is to obtain the approximate solution f_n on a mesh $\{t_{n,j}\}_{j=1}^{n}$ by solving a system of n linear algebraic equations

$$\sum_{j=1}^{n} \left[\delta_{ij} + K(t_{n,i}, t_{n,j}) w_{n,j}\right] f_n(t_{n,j}) = y(t_{n,i}). \tag{2.18}$$

From these coefficients the function $f_n(s)$ is uniquely defined. Equation (2.17) is a natural interpolation formula for the n coefficients $\{f_n(t_{n,j})\}_{j=1}^{n}$. The rate of convergence of the Nyström method is limited by the rate at which $\mathscr{K}_n f$ approaches $\mathscr{K}$f. A standard error analysis shows that

$$\|f - f_n\| \leqslant \left\|(I + \mathscr{K}_n)^{-1}\right\| \|(\mathscr{K} - \mathscr{K}_n) f\|, \tag{2.19}$$

where the norm is the uniform norm and $\left\|(I + \mathscr{K}_n)^{-1}\right\|$ is bounded. See Atkinson [2] for a theoretical development of this result.

For $\mathscr{K}$ continuous and sufficiently smooth we can use equation (2.19) and equation (2.8) of the convergence theorem to obtain a convergence rate

$$\|f - f_n\| \sim O(h_z^{l+1}). \tag{2.20}$$

Therefore, in the cases of linear, quadratic, cubic, and quartic splines we expect the Nyström method using Gauss quadrature to give errors of order 2, 3, 4 and 5 respectively.

A number of iterative variants of the Nyström method are available and have been studied by Atkinson [2,3]. For the purpose of our calculations we adopt the method proposed by Brakhage [6], which makes use of the inverse operator $(I + \mathscr{K}_m)^{-1}$, with $m < n$.

We rewrite the operator form of equation (2.17) as

$$(I + \mathscr{K}_m) f_n = y - (\mathscr{K}_n - \mathscr{K}_m) y + (\mathscr{K}_n - \mathscr{K}_m) \mathscr{K}_n f_n, \tag{2.21}$$

where $m < n$. Given an approximate solution $f_n^{(0)}$, the equation (2.2) may be solved iteratively. In a form suitable for computation the iterative equation becomes [2]

$$f_n^{(p+1)}(s) = f_n^{(p)}(s) + \zeta^{(p)}(s) + \gamma^{(p)}(s), \tag{2.22}$$

where

$$\zeta^{(p)}(s) = y(s) - f_n^{(p)}(s) - \sum_{j=1}^{n} K(s, t_{n,j}) f_n^{(p)}(t_{n,j}) w_{n,j}, \tag{2.23}$$

$$\gamma^{(p)}(s) = -\sum_{j=1}^{m} K(s, t_{m,j}) \gamma^{(p)}(t_{m,j}) w_{m,j} - \sum_{j=1}^{n} K(s, t_{n,j}) \zeta^{(p)}(t_{n,j}) w_{n,j}, \tag{2.24}$$

and the coefficients $\{\gamma^{(p)}(t_{m,j})\}_{j=1}^{m}$ are obtained by solving the system of m linear algebraic equations

$$\sum_{j=1}^{m} \left[\delta_{ij} + K(t_{m,i}, t_{m,j}) w_{m,j}\right] \gamma^{(p)}(t_{m,j}) = -\sum_{j=1}^{n} K(t_{m,i}, t_{n,j}) \zeta^{(p)}(t_{n,j}) w_{n,j}. \tag{2.25}$$

The iterative scheme is guaranteed to converge if m is sufficiently large [2].

3. Integral equations for two-body scattering

This section describes an integral equation of the form (1.1) for the quantum scattering of two mutually interacting particles. The partial wave two-body k-matrix $M(q, \kappa)$ is a solution of the Lippmann–Schwinger integral equation

$$M(q, \kappa) = v(q, \kappa) - \frac{2}{\pi} P \int_0^\infty v(q, q') M(q', \kappa) \frac{q'^2 \, dq'}{q'^2 - \kappa^2}. \tag{3.1}$$

Here, $v(q, q')$ is the Fourier transformed potential, and $\kappa \geqslant 0$ denotes the on-shell momentum in the center of mass frame. The function $v(q, q')$ falls off sufficiently rapidly that the integral equation (3.1) is Fredholm. The integral in equation (3.1) is evaluated with respect to a principal value prescription. The function $M(q, \kappa)$ is real valued and can be expressed in terms of a phase shift $\delta(\kappa)$ by

$$M(\kappa, \kappa) = -[\kappa \cot \delta(\kappa)]^{-1}. \tag{3.2}$$

We notice that for momenta $\kappa > 0$ the equation (3.1) does not have a continuous kernel. The principal value of the improper integral may, however, be evaluated using standard numerical techniques [16]. The method we employ is to subtract the singularity [8]. Equation (3.1) becomes

$$M(q, \kappa) = v(q, \kappa) - \frac{2}{\pi}\int_0^\infty \frac{\left[q'^2 v(q, q')M(q', \kappa) - \kappa^2 v(q, \kappa)M(\kappa, \kappa)\right]\mathrm{d}q'}{q'^2 - \kappa^2}. \tag{3.3}$$

It now remains to apply the Gauss formula to equation (3.3). Since our quadrature formula is defined on the interval $[-1, 1]$, we must introduce a suitable transformation of the points $\{t_{n,j}\}_{j=1}^n$ and weights $\{w_{n,j}\}_{j=1}^n$. For this purpose we choose

$$q_{n,j} = \eta\left(\frac{1 + t_{n,j}}{1 - t_{n,j}}\right), \qquad \nu_{n,j} = \frac{2\eta w_{n,j}}{(1 - t_{n,j})^2}, \tag{3.4}$$

where η is a constant scale parameter. Application of the transformed quadrature formula to equation (3.3) gives

$$M_n(q, \kappa) = v(q, \kappa) - \frac{2}{\pi}\sum_{j=1}^{n} \frac{q_{n,j}^2 \nu_{n,j}}{q_{n,j}^2 - \kappa^2} v(q, q_{n,j}) M_n(q_{n,j}, \kappa)$$

$$+ \frac{2}{\pi}\sum_{k=1}^{n} \frac{\kappa^2 \nu_{n,k}}{q_{n,k}^2 - \kappa^2} v(q, \kappa) M_n(\kappa, \kappa), \tag{3.5}$$

where M_n is the approximate solution using the Nyström method. In addition to the coefficients $\{M_n(q_{n,j}, \kappa)\}_{j=1}^n$, the interpolatory formula also requires the on-shell value $M_n(\kappa, \kappa)$. A method devised by Haftel and Tabakin [10] is to construct a system of $n + 1$ algebraic equations where κ is the $(n + 1)$th point. (It is assumed that κ is not equal to any of the transformed quadrature points $\{q_{n,j}\}_{i=1}^n$.)

Let

$$p_{n+1,j} = \begin{cases} q_{n,j}, & 1 \leqslant j \leqslant n, \\ \kappa, & j = n + 1, \end{cases}$$

$$W_{n+1,j} = \begin{cases} \dfrac{q_{n,j}^2 \nu_{n,j}}{q_{n,j}^2 - \kappa^2}, & 1 \leqslant j \leqslant n, \\ \kappa^2 \displaystyle\sum_{k=1}^{m} \frac{\nu_{n,k}}{q_{n,k}^2 - \kappa^2}, & j = n + 1. \end{cases} \tag{3.6}$$

In this notation equation (3.5) becomes

$$M_n(q, \kappa) = v(q, \kappa) - \frac{2}{\pi}\sum_{j=1}^{n+1} W_{n+1,j} v(q, p_{n+1,j}) M_n(p_{n+1,j}, \kappa). \tag{3.7}$$

The modified Nyström method suggested by the work of Haftel and Tabakin is to solve the system of $n + 1$ linear algebraic equations

$$\sum_{j=1}^{n+1}\left[\delta_{ij} + \frac{2}{\pi} W_{n+1,j} v(p_{n+1,i}, p_{n+1,j})\right] M_n(p_{n+1,j}, \kappa) = v(p_{n+1,i}, \kappa). \tag{3.8}$$

4. Numerical results and discussion

In order to test the performance of the Nyström method using a Gauss quadrature for splines we have solved the integral equations numerically. For this purpose we have chosen splines of degree $l = 1, 2, 3$ and 4 with uniformly spaced knots on the interval $[-1, 1]$. For evaluating the B-splines we use the stable algorithm of Cox [5] and De Boor [4].

Convergence rates of the approximation for given spline functions are checked numerically by halving the grid size. If the solution of the integral equations is not known, then we calculate the convergence rate as follows: Let $f(h)$ be the approximate solution obtained with a grid size h. Then

$$f(h) \approx f + ch^{\beta}, \tag{4.1}$$

where f is the unknown solution, c is a constant and β is the convergence rate. We half the grid size twice to obtain the estimate

$$\beta \approx [\ln(2)]^{-1} \ln\left[\frac{f(h) - f(\frac{1}{2}h)}{f(\frac{1}{2}h) - f(\frac{1}{4}h)}\right]. \tag{4.2}$$

Equation (4.2) gives an indication of the rate of convergence, provided h is sufficiently small and the calculated values are monotone.

First, we consider some computational aspects of the Gauss quadrature for splines. Solving the system of moment equations (2.5)–(2.6) is the 'brute force' method. The equations are solved using a general purpose non-linear system solver. Table 1 shows the points and weights of a 20-point Gauss quadrature formula calculated using cubic polynomial splines. The remaining points and weights are obtained by symmetry (see equation (2.4)). For general l we observe that towards the center of the integration interval $[-1, 1]$ (i) the quadrature points tend to be equidistant at an interval of $4/(2n - l)$, and (ii) the weights tend to be equal to $4/(2n - l)$. (Note that in the case of cubic splines $4/(2n - 3) = 0.108108108108\ldots$ and $2/(2n - 3) = 0.054054054054\ldots$.) This observation leads to a more efficient way of constructing our n-point Gauss quadrature formula without solving a non-linear system. The method is described in the Appendix.

Table 1
Points and weights of the 20-point Gauss quadrature for splines

k	$-t_{20,k}$	$w_{20,k}$
1	−0.98186561675920	0.04605280116483
2	−0.91068073290352	0.09129068258111
3	−0.80999835643869	0.10608287371966
4	−0.70263669551663	0.10793959242049
5	−0.59458934105903	0.10809466968612
6	−0.48648606905546	0.10810704016331
7	−0.37837834521492	0.10810802326251
8	−0.27027026763558	0.10810810136746
9	−0.16216216195294	0.10801810757237
10	−0.05405405403860	0.10810810806214

Table 2
Errors for spline-degenerate kernel method

l	$1/h = 6$	12	24	48
1	2.3 (−2)	5.8 (−3)	1.5 (−3)	3.7 (−4)
2	1.4 (−4)	8.7 (−6)	5.5 (−7)	3.4 (−8)
3	5.6 (−4)	3.5 (−5)	2.2 (−6)	1.4 (−7)
4	4.2 (−6)	6.6 (−8)	1.0 (−9)	1.6 (−11)

Table 3
Errors for Nyström method with spline quadrature

l	$1/h = 6$	12	24	48
1	7.3 (−3)	1.8 (−3)	4.5 (−4)	1.1 (−4)
2	1.4 (−4)	8.4 (−6)	5.2 (−7)	3.2 (−8)
3	3.2 (−5)	2.1 (−6)	1.3 (−7)	8.0 (−9)
4	1.3 (−6)	2.1 (−8)	4.9 (−10)	1.6 (−8)

Table 4
Errors for Nyström method with Gauss quadrature for splines

l	$1/h = 6$	12	24	48
1	3.7 (−3)	1.0 (−3)	2.4 (−4)	5.9 (−5)
2	3.8 (−6)	1.1 (−6)	9.2 (−8)	6.2 (−9)
3	4.2 (−5)	2.3 (−6)	1.3 (−7)	7.7 (−9)
4	1.8 (−6)	3.3 (−8)	5.6 (−10)	8.9 (−12)

In order to test our numerical algorithm for solving integral equations with spline-Gauss quadrature we first solve a simple test problem. Our results are compared with those of a degenerate kernel method [11] and also a Nyström method using ordinary spline quadrature [19]. The test problem [11, example 6.1] is the homogeneous integral equation

$$\lambda\psi(s) = \int_0^1 \sin\left[\tfrac{1}{2}\pi(s+t)\right]\psi(t)\,\mathrm{d}t. \tag{4.3}$$

The largest eigenvalue for this problem is $0.5 + \pi^{-1} = 0.81830989$.

Tables 2–4 show the error in the eigenvalue for the three different methods of solving equation (4.3) based on splines. In Table 2 a degenerate kernel method using the algorithm of Hämmerlin and Schumaker [11] was used to find the approximate eigenvalue. In table 3 a Nyström method using ordinary spline quadrature was used. In the case of spline quadrature we have placed the quadrature points on the position of the knots $\{z_i\}_{i=1}^{r}$ and at the end points -1 and $+1$. Additional points, as required, are placed in the end intervals $[-1, z_1]$ and $[z_r, 1]$. The weights tend to oscillate for even-degree splines, and this is reflected in the non-monotonic behaviour of the error for quartics.

Lastly, Table 4 shows the error in the eigenvalue obtained from a Nyström method using

Table 5
Rate of convergence

l	Table 2	Table 3	Table 4
1	2.0	2.0	2.0
2	4.0	4.0	3.9
3	4.0	4.0	4.1
4	6.0	Not monotone	6.0

Gauss quadrature for splines. In this case the number of quadrature terms n is half the number of spline basis functions. Hence, for splines of degree l, the grid spacing h is given by

$$1/h = 2n - l. \tag{4.4}$$

Formula (4.4) gives a result that if we halve the grid size for splines of odd degree, then n takes on half-integer values. Therefore, in the case of linear and cubic splines we have taken the nearest whole number of Gauss points for our quadrature formula. For sufficiently large n this approximation is expected to give only a small change in our rate of convergence estimate. Table 5 shows a numerical rate of convergence calculated from Table 2–4. The results for splines of even degree ($l = 2$, 4) show superconvergence, meaning that the rate of convergence is higher than expected.

The results tabulated in Tables 2–5 show that for splines of a given degree similar accuracy and rate of convergence are obtained for all three methods. The advantage of a Nyström method using Gauss quadrature is that we obtain this accuracy by solving a smaller system or equations. We now turn to the Lippmann–Schwinger integral equation (3.1) and an application of the modified Nyström method using Gauss quadrature for splines. A problem taken from nuclear physics is to calculate the phase shift $\delta(\kappa)$, defined by equation (3.2), for the Reid $^1S_0$ soft core potential [18]. In momentum space this potential has the form

$$v(q, q') = \frac{1}{4\mu_1 qq'} \sum_{i=1}^{3} V_i \ln\left[\frac{(q+q')^2 + \mu_i^2}{(q-q')^2 + \mu_i^2}\right], \tag{4.5}$$

where $\mu_1 = 0.7$ fm^{-1}, $\mu_2 = 4\mu_1$, $\mu_3 = 7\mu_1$, $V_1 = -10.463$ MeV · fm^{-3}, $V_2 = -1650.6$ MeV · fm^{-3} and $V_3 = 6484.2$ MeV · fm^{-3}. We take $\hbar^2/m = 41.47$ MeV · fm^2, where m is the nucleon mass. We fix the scattering energy at 24 MeV in the center of mass frame, and choose a scale parameter $\eta = 10$. Table 6 shows the approximate values of the phase shift $\delta(\kappa)$ calculated with a modified Nyström method. The results are seen to converge as we increase the number of Gauss points $n = \frac{1}{2}(1/h + l)$. The estimated rate of convergence β is shown in Table 7.

Table 6
Phase shift (deg) for the Reid $^1S_0$ potential at 24 MeV scattering energy

l	$1/h = 12$	24	48	96
1	49.69198	39.05124	39.22125	39.22491
2	36.70978	39.31686	39.22492	39.22426
3	37.12772	39.39438	39.22596	39.22427
4	42.35817	39.26045	39.22556	39.22426

Table 7
Estimated rates of convergence

l	β
1	5.5
2	7.1
3	6.6
4	4.7

Table 8
Brakhage iterative method

p	$l=1$	2	3	4
1	39.22013	39.22446	39.22545	39.22546
2	39.22126	39.22493	39.22596	39.22555
3	39.22125	39.22492	39.22596	39.22555

We have applied the Brakhage iterative method to this problem. Table 8 shows the approximate phase shift $\delta(\kappa)$ after p iterations using an m-mesh with $1/h = 24$ and an n-mesh with $1/h = 48$. The starting value is an approximate solution M_m obtained using the Nyström method. We find that after two iterations ($p = 2$) the Brakhage iterative method converges on an approximate value of $\delta(\kappa)$ that is close to the solution of the Nyström method using the large n-mesh.

We have shown by numerical example that our approximation method yields accurate results for a problem taken from quantum scattering. Our method combines the good interpolation properties of splines with the simplicity of a Nyström method using Gauss quadrature. For the problem we have considered the Brakhage iterative method may be used to improve the accuracy of the approximate solution without the need to solve a large linear system.

Acknowledgement

This paper is work done as part of a Ph.D. thesis by one of the authors (LP) under the direction of Professor D.P. Laurie of the Department of Mathematics and Applied Mathematics at the Potchefstroom University for CHE.

Appendix. An algorithm for constructing spline-Gauss quadrature

For simplicity we consider only the case of cubic splines. The 'brute force' method yields the following results.

(i) $|\Delta t_{n,k}| \to 4/(2n-3)$ as $k \to \lfloor \frac{1}{2}n \rfloor$, (A.1)

(ii) $t_{n,\lfloor n/2 \rfloor} \approx -2/(2n-3)$ and for odd n $t_{n,(n+1)/2} = 0$, (A.2)

(iii) $w_{n,k} \to 4/(2n-3)$ as $k \to \lfloor \frac{1}{2}n \rfloor$. (A.3)

These results suggest the transformation

$$y_{n,k} = -(n-2k+1) - (n-\tfrac{3}{2})t_{n,k}, \tag{A.4}$$

$$u_{n,k} = 2 - (n-\tfrac{3}{2})w_{n,k}, \quad k = 1, 2, \ldots, \lfloor \tfrac{1}{2}n \rfloor, \tag{A.5}$$

where $y_{n,k}$ and $u_{n,k}$ are the difference between the limiting and actual values of $t_{n,k}$ and $w_{n,k}$ respectively on the transformed interval $[-n+\frac{3}{2}, n-\frac{3}{2}]$. Thus for fixed n,

$$\lim_{k \to \lfloor n/2 \rfloor} y_{n,k} = -1 - (n-\tfrac{3}{2})t_{n,\lfloor n/2 \rfloor}, \tag{A.6}$$

$$\lim_{k \to \lfloor n/2 \rfloor} u_{n,k} = 2 - (n-\tfrac{3}{2})w_{n,\lfloor n/2 \rfloor}, \tag{A.7}$$

and

$$\lim_{k\to[n/2]} y_{n,k} \to 0, \qquad \lim_{k\to[n/2]} u_{n,k} \to 0 \quad \text{as } n \to \infty. \tag{A.8}$$

We also observe that for fixed k.

$$\lim_{n\to\infty} y_{n,k} = y_k, \qquad \lim_{n\to\infty} u_{n,k} = u_k. \tag{A.9}$$

These observations form the basis of an algorithm for constructing our n-point gauss quadrature formula for cubic splines for arbitrary n. This algorithm does not entail the solution of a system of equations, but involves asymptotic expansions for $y_{n,k}$ and $u_{n,k}$.

Rewriting the system (2.5)–(2.6) in terms of the cubic B-spline basis, we obtain

$$B_i(t) = \tfrac{1}{4}\big[(t-z_{i-2})_+^3 - 4(t-z_{i-1})_+^3 + 6(t-z_i)_+^3 - 4(t-z_{i+1})_+^3 + (t-z_{i+2})_+^3\big],$$
$$i = -1, 0, 1, \ldots, 2n-2, \tag{A.10}$$

for $\{1,\ t,\ t^2,\ t^3,\ (t-z_1)_+^3, \ldots, (t-z_{2n-4})_+^3\}$. Applying the transformation (A.4)–(A.5), and abbreviating $y_{n,k}$ by y_k and $u_{n,k}$ by u_k, we obtain

$$\begin{aligned}
&(2-u_1)(8y_1^3 + 36y_1^2 + 54y_1 + 27) = 2,\\
&(2-u_1)(-24y_1^3 - 84y_1^2 - 66y_1 + 17) + (2-u_2)(8y_2^3 + 12y_2^2 + 6y_2 + 1) = 24,\\
&(2-u_1)(24y_1^3 + 60y_1^2 + 18y_1 + 5) + (2-u_2)(-24y_2^3 - 12y_2^2 + 30y_2 + 23) = 46,\\
&(2-u_1)(-8y_1^3 - 12y_1^2 - 6y_1 - 1) + (2-u_2)(24y_2^3 - 12y_2^2 - 30y_2 + 23)\\
&\quad + (2-u_3)(8y_3^3 - 12y_3^2 + 6y_3 + 1) = 48,\\
&(2-u_2)(-8y_2^3 + 12y_2^2 - 6y_2 + 1) + (2-u_3)(-24y_3^3 - 12y_3^2 + 30y_3 + 23) = 48,\\
&(2-u_k)(24y_k^3 - 12y_k^2 - 30y_k + 23) + (2-u_{k+1})(8y_{k+1}^3 + 12y_{k+1}^2 + 6y_{k+1} + 1) = 48,\\
&(2-u_k)(-8y_k^3 + 12y_k^2 - 6y_k + 1)\\
&\quad + (2-u_{k+1})(-24y_{k+1}^3 - 12y_{k+1}^2 + 30y_{k+1} + 23) = 48,\\
&\quad k = 3, 4, 5, \ldots, [\tfrac{1}{2}n] - 1,\\
&(2-u_{n/2})(4y_{n/2}^3 - 9y_{n/2} + 6) = 12.
\end{aligned} \tag{A.11}$$

For odd n the last equation is replaced by the equations

$$\begin{aligned}
&(2-u_k)(24y_k^3 - 12y_k^2 - 30y_k + 23) - u_{k+1} = 46,\\
&(2-u_k)(-8y_k^3 + 12y_k^2 - 6y_k + 1) - 23u_{k+1} = 2,
\end{aligned} \tag{A.12}$$

where $k = [\frac{1}{2}n]$.

The system (A.11) comprises five equations describing the behaviour of y_k and u_k, $k = 1, 2, 3$ at the boundary -1, followed by a pair of typical equations in y_k, y_{k+1}, u_k and u_{k+1}, occurring $[\frac{1}{2}n] - 3$ times, and one or two equations describing the symmetric behaviour of y_k and u_k, $k = [\frac{1}{2}n]$, $[\frac{1}{2}n] + 1$, at the origin. For large n the pair of typical equations dominate the system, and may be used to obtain asymptotic expansions for y_k and u_k for arbitrary n.

We assume that y_k, y_{k+1}, y_{k+1}, u_k and u_{k+1} are $O(\epsilon)$ and ignore $O(\epsilon^2)$ plus higher order terms. From the typical equation of (A.11) we obtain

$$y_{k+1} = \tfrac{19}{3}y_k + \tfrac{22}{9}u_k + O(\epsilon^2), \qquad u_{k+1} = 16y_k + \tfrac{19}{3}u_k + O(\epsilon^2). \tag{A.13}$$

By solving the two-dimensional homogeneous first-order difference system (A.13) we obtain the first-order terms $u_k^{(0)}$ and $y_k^{(0)}$ in the asymptotic expansions for u_k and y_k respectively, namely

$$u_k^{(0)} = \tfrac{1}{2}\lambda^k u_0 - \left(6\sqrt{22}/11\right)\lambda^k y_0, \qquad y_k^{(0)} = -\tfrac{1}{24}\sqrt{22}\,\lambda^k u_0 + \tfrac{1}{2}\lambda^k y_0, \tag{A.14}$$

where λ, and λ^{-1} are the eigenvalues of the matrix

$$\begin{bmatrix} \frac{19}{3} & 16 \\ \frac{22}{9} & \frac{19}{3} \end{bmatrix}, \tag{A,15}$$

u_0 and y_0 are known starting values.

Second-order and further terms in these asymptotic expansions may be found by ignoring $O(\epsilon^3)$ plus higher order terms and proceeding as above.

References

[1] A. Alaylioglu, D.S. Lubinsky and D. Eyre, Product integration of logarithmic singular integrands based on cubic splines, *J. Comp. Appl. Math.* **11** (1984) 353–366.

[2] K.E. Atkinson, *A Survey of Numerical Methods for the Solution of Fredholm Integral Equations of the Second kind* (SIAM, Philadelphia, 1976).

[3] K.E. Atkinson, Iterative variants of the Nyström method for the numerical solution of integral equations, *Numer. Math.* **22** (1973) 17–31.

[4] C. de Boor, *A Practical Guide to Splines* (Springer, New York, 1978).

[5] C. de Boor, On Calculating with B-splines, *J. Approx. Theory* **6** (1972) 50–62.

[6] H. Brakhage, Über die numerische Behandlung von Integralgleichungen nach der Quadraturformelmethode, *Numer. Math.* **2** (1960) 183–196.

[7] M.G. Cox, The numerical evaluation of B-splines, *J. Inst. Math. Appl.* **10** (1972) 134–149.

[8] P.J. Davis and P.Rabinowitz, *Methods of Numerical Integration* (Academic Press, New York, 1975).

[9] W. Glockle, G. Hasberg and A.R. Neghabian, Numerical treatment of few-body equations in momentum space by spline methods, *Z. Phys. A* **305** (1982) 217–221.

[10] M.I. Haftel and F. Tabakin, Nucleon saturation and smoothness of nucleon-nucleon potentials, *Nucl. Phys. A* **158** (1970) 1–42.

[11] G. Hämmerlin and L.L. Schumaker, Procedures for kernel approximation and solution of Fredholm integral equations of the second kind, *Numer. Math.* **34** (1980) 125–141.

[12] J. Horacek and L. Malina, Cubic splines and the Lippmann-Schwinger equation, *Czech. J. Phys. B* **27** (1977) 1–6.

[13] S. Karlin and W.J. Studden, *Tchebyscheff Systems: with Applications in Analysis and Statistics* (Interscience Publications, New York, 1966).

[14] C.A. Micchelli and A. Pinkus. Moment theory for weak Chebyshev systems with applications to monosplines, quadrature formulae and best one-sided L^1-approximation by spline functions with fixed knots, *SIAM J. Math. Anal.* **8** (1977) 206–230.

[15] A.N. Netravali and R.J.P. DeFigueiredo, Spline Approximation to the solution of the linear Fredholm integral equation of the second kind, *SIAM. J. Numer. Anal.* **11** (1974) 538–549.

[16] B. Noble and S. Beighton, Error estimates for three methods of evaluating Cauchy principal value integrals, *J. Inst. Maths. Applics.* **26** (1980) 431–446.

[17] E.J. Nyström, Uber die praktische Auflosung von Integralgleichungen mit Anwendungen auf Randwertaufgaben, *Acta Math.* **54** (1930) 185–204.

[18] R.V. Reid Jr., Local phenomenological nucleon-nucleon potentials, *Annals of Phys.* **50** (1968) 411–448.

[19] I.J. Schoenberg, *Cardinal Spline Interpolation* (SIAM, Philadelphia, 1973).

[20] A.H. Stroud and D. Secrest, *Gaussian Quadrature Formulas* (Prentice-Hall, Englewood Cliffs, NJ, 1966).